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Ring Test with the Models LEACHP, PRZM-2 and VARLEACH: Variability between Model Users in Prediction of Pesticide Leaching Using a Standard Data Set

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Abstract: A ring test was carried out with three mathematical models for pesticide leaching to compare predictions from a number of modellers for a single field experiment when using the same model. The exercise sought to investigate the level of variation, if any, in model output introduced by user-dependent subjectivity during selection of input parameters. Five modellers were given a full description of a field experiment carried out in the UK to determine the leaching potential of a novel pesticide and then used the models LEACHP, PRZM-2 and VARLEACH to predict concentrations of pesticide in soil water at 1 m depth and in soil for a 1 m profile 220 days after application. Agreement with observed results was generally best for LEACHP and worst for VARLEACH, but no two sets of predicted results for a given model were exactly the same, even for the simple model VARLEACH. Differences between simulations with the same model were attributed to a number of input parameters which could not be derived from the experimental information provided and thus introduced subjectivity into the modelling process. The parameters identified included dispersivity, initial soil conditions and factors determining the rate of pesticide degradation. Differences between output data with the same model were of a similar order of magnitude to the variation associated with field measurements and were generally smaller than the discrepancies between observed and predicted data. User-dependence of modelling has not previously been considered, but should be an important component in assessing model output and in evaluating the validity and use of a given programme. Model development should seek to reduce subjectivity in selection of input parameters and improve the guidance available to users where subjectivity cannot be eliminated.

Key words: mathematical models, pesticide leaching, user-dependence, parameter selection

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1 INTRODUCTION

Mathematical models are used extensively to simulate the fate and behaviour of compounds in the environment. Formerly, models were used principally as research or management tools to aid experimental design and interpretation or agricultural management at the local scale. Increasingly, however, models are being used predictively to facilitate decision-making by regulatory authorities and the industrial sector. Assurance of quality in such modelling exercises is essential and much work is in progress to evaluate the predictive ability of mathematical models, validate subroutines and improve documentation of models and modelling procedures.[1–3] Evaluation of models has concentrated upon the comparative ability of a range of models to simulate standard datasets, with the aim that the best models or parts of models be recommended for use in a given situation. To date, no work has focused on the reproducibility of results from any given model when used predictively by a range of workers to simulate the same scenario. Such inter-laboratory ring tests are a routine procedure used to assess the level of confidence associated with results from any novel analytical or sampling technique, but have not been extended to the subject of modelling fate and behaviour in the environment. This paper will present simulation results for a field experiment prepared by five experienced modellers using three established pesticide leaching models, LEACHP,[4] PRZM-2[5] and VARLEACH.[6]

2 EXPERIMENTAL DETAILS

A field experiment was established in the autumn of 1993 by Monsanto Agricultural Company in Derbyshire, UK, to investigate the potential for leaching and accumulation of a research agrochemical which remains anonymous for the purpose of this ring test. The experimental site was located on a coarse loamy gleyic brown earth soil of the Arrow series which is a sandy loam over loamy sand at depth. Table 1 details the soil characteristics.

On 2 November 1993, winter wheat (*Triticum aestivum* L *cv.* Riband) seed-treated with the test chemical at a rate of 1 g AI kg^{-1} seed was sown using a Pneumatic Accord seed drill with a 4-m operating width at a rate of 200 kg seed ha^{-1} to give a total application of the test chemical of 200 g AI ha^{-1}. The site was subsequently instrumented by installing 10 soil water suction samplers to a depth of 100 cm. These suction samplers allowed soil water to be collected from the appropriate soil depth during periods when the soil was at or near to field capacity and their design has been previously described in detail.[7] Nine of the suction samplers drew water from the area treated with the test chemical and the remaining sampler drew water from an untreated area and acted as a control. Soil-water samples were collected from the site at fortnightly intervals for the first six weeks after application of the test substance and subsequently monthly. In addition, water sampling was triggered by rainfall events $\geqq 10$ mm over a 24-hour period or $\geqq 15$ mm over a 48-hour period.

Soil-water samples were stored individually in sealed glass bottles and transferred to Hazleton UK Limited, Harrogate, North Yorkshire, UK where they were frozen at $-15°C$. Samples were extracted by partitioning into dichloromethane, cleaned up by reverse-phase HPLC and then analysed by GC with electron capture detection. The limit of determination for the test chemical in soil water was 0·1 μg $litre^{-1}$ and recovery from six samples spiked to 0·5 μg $litre^{-1}$ ranged from 78 to 113% with a mean of 97%.

In order to investigate soil dissipation rates for the test chemical, soil samples were taken at regular intervals to 30 cm depth as three blocks 30 × 14 × 10 cm deep. On 8 June 1994, the depth of soil sampling was extended to 1 m in order to aid interpretation of soil water data. Three pits were dug to this depth and 10 blocks each 10 cm deep were taken from one side of each pit. Soil samples were again stored frozen until extraction and analysis at Hazleton UK Limited. Soil was extracted by shaking with aqueous acetonitrile, partitioning into dichloromethane and cleaning-up on a florisil column before analysis by GC with electron capture detection. The limit of determination for the test chemical in soil was 0·5 μg kg^{-1} and recovery from six samples spiked to 0·5 mg kg^{-1} ranged from 74 to 99% with a mean of 90%.

Rainfall and other weather parameters were measured at the Sutton Bonington campus of Nottingham

TABLE 1
Characteristics of the Soil at the Field Site

Depth (cm)	C_{org} (%)	*pH*	*Bulk density* (cm^3 g^{-1})	*Sand* (%)	*Silt* (%)	*Clay* (%)	*Water content* (g g^{-1}) 5 kPa	1500 kPa
0–30	1·3	6·6	1·50	69·1	20·5	10·4	20·2	8·9
30–48	0·5	6·5	1·55	72·4	17·7	9·9	16·1	7·2
48–82	0·3	6·5	1·56	77·1	15·3	7·6	16·2	7·4
82–110	0·1	6·2	1·54	89·9	6·3	3·8	19·2	2·7

TABLE 2
Monthly Means of Daily Temperatures and Total Monthly Rainfall for Sutton Bonington, November 1993–June 1994

Month	*Maximum temperature (°C)*	*Minimum temperature (°C)*	*Rainfall (mm)*
November 1993	7·1	2·6	57·1
December 1993	8·5	2·6	93·7
January 1994	7·9	2·3	76·1
February 1994	6·0	0·1	47·3
March 1994	11·4	4·4	64·3
April 1994	12·3	4·6	32·3
May 1994	14·2	6·0	53·7
June 1994	19·8	9·5	8·2

University (approximately 5 km from the experimental site) and these are summarised for the experimental period in Table 2.

3 MODELLING

The authors participated in a ring test to investigate the reproducibility of model results, which followed the principles of a laboratory ring test to assess analytical techniques or laboratory test methods. The modellers at institutes in France, Germany and Italy, and two in the UK, received a description of the field experiment. Apart from the originator of the test, none of the other modellers received any information about the results obtained in the experiment and each was asked to use the pesticide leaching models LEACHP, PRZM-2 and VARLEACH to predict the experimental results.

The experimental description circulated to the modellers is outlined in Table 3. The data provided followed a standard layout developed for a European experimental database created to facilitate model evaluation.[8] All of the values apart from weather and properties of the chemical were measured at the site. A representative value for the organic carbon partition coefficient and the water solubility and vapour pressure of the chemical had previously been determined using standard laboratory methods to be 100 ml g^{-1}, 139 mg $litre^{-1}$ and 0·79 mPa, respectively. The field half-life given for modelling purposes was derived from the field experiment. This means that care should be taken in comparing observed and predicted data as they are not fully independent, but this is not significant for the ring test which aimed to determine the reproducibility of simulations performed by a number of different modellers for the same experiment. All three of the models used allow pesticide to be incorporated to a specified depth, but do not allow pesticide to be banded at a single depth below the surface. Hence the application of the test chemical as a seed treatment was ignored for modelling purposes and modellers were asked simply to model a surface application of test compound at the equivalent rate. All simulations with VARLEACH assume incorporation of pesticide to a fixed depth of 1 cm. Weather data were provided covering the experimental period and for ten months before treatment to give modellers the opportunity of an equilibration period for the simulations if desired.

All modellers used the same versions of three established models—LEACHP 3.1, PRZM-2 Version 2.0 and VARLEACH 2.0 (see Table 4). PRZM-2 and LEACHP have been the most widely used models to date for predicting the movement of pesticides through soil, whilst VARLEACH is a derivative of CALF[9] and has been extensively used in the UK and increasingly in Europe. Each modeller worked within a user-friendly interface called MARVEL (version 4.0) which has been developed to facilitate the use of these three models. The interface facilitates parameter selection and entry by providing initial sample values, redundant parameter exclusion and automatic rejection of input parameters outside

TABLE 3
Overview of Experimental Description Provided to Modellers in the Ring Test

Parameter category	*Information provided*
Site	Location, altitude, latitude, slope, minimum depth to water table, sampling methodology
Soil	Subgroup and series, organic carbon content, particle size distribution, pH, bulk density, water content at 5 kPa and 1500 kPa, microbial biomass
Crop	Crop type, dates of sowing and harvesting
Pesticide application	Application rate, date and method[a]
Pesticide properties	Water solubility, K_{oc}, field half-life[a], vapour pressure
Weather	Daily maximum and minimum temperatures and rainfall for the period 1 Jan. 1993–8 June 1994[b]

[a] See text for qualification.
[b] Pan evaporation data measured at Wellesbourne, Warwickshire for the period 1 Nov. 1993–8 June 1994 was additionally provided for simulations with VARLEACH.

specified ranges. These ranges were often specially defined with the aid of the model authors for the interface. MARVEL also provides a comprehensive help menu taken from the users' manual for PRZM-2, developed from the more limited help available with the manual for LEACHP, and written specially for this application for VARLEACH. For the inexperienced user, it is thus likely that modelling within the constraints of the MARVEL interface would significantly decrease the user-dependent variation introduced into any given simulation. For the present exercise, the main effects were to ensure-that all modellers started with the same set of default values from which to begin changing inputs to best simulate the field experiment and to minimise the likelihood of mistakes during entry of parameters. The user-dependent variability between simulations described in this paper may thus underestimate the variability if the models were used independent of the interface. The extent of the underestimation will dependent on the quality of guidance given in the users' manual, the availability of the parameters needed to carry out a simulation, and the ease with which input files are constructed to reflect the selected parameters.

LEACHP is a mechanistic model which is typical of research models. PRZM-2 is a management model developed in the US and belongs to a simpler model group, but nevertheless requires a wide range of parameters and factors to allow simulations to be run. VARLEACH is the simplest of the three models, requiring only readily measured data as input and being based upon a rigorous description of pesticide degradation and a simple subroutine to simulate water and solute movement through soil. A brief overview of the most important features of each model is given in Table 4, but full descriptions of the model characteristics can be found in the references cited.

Each of the modellers was asked to predict the concentration of the test chemical in soil water at 1 m depth collected on 14 dates between 10 November 1993 and 23 May 1994 and to predict bulk residues of the parent compound in soil at 10-cm increments on 8 June 1994.

4 RESULTS AND DISCUSSION

The results observed in the field experiment are compared with the five model predictions from all three models in Table 5 and in Figs 1 and 2 (note simulations 1–5 are not in the same order as the list of authors, but the numbering is consistent across all three models). The field results showed a moderate amount of leaching of the test chemical over the winter and spring of 1993/94. Breakthrough of pesticide at 1 m depth occurred at

TABLE 4
Overview of the Three Mathematical Models Used for the Ring Test

Property	*LEACHP 3·1*	*PRZM-2·0*	*VARLEACH 2·0*
Latest reference	Hutson & Wagenet, 1992[4]	Mullins *et al.*, 1994[5]	Walker & Hollis, 1994[6]
First developed	1987	1984	1982
Water description	Richards' equation	'Tipping-bucket'	Two-region tipping bucket
Bypass flow	Not described	Not described	Not described
Runoff/erosion	No	Yes	No
Solute transport	Convection-dispersion equation	Convection-dispersion equation	Daily equilibration
Dispersion	Required as input	Can be input or fixed by layer depth in model	Fixed by mobile-immobile water separation and layer depth in model
Water content-conductivity relationships	Calculated from basic soil data or retentivity curve according to Campbell's equation	Water contents required as input; conductivity not required	Water contents required as input; conductivity not required
Plant growth	Yes	Yes	No
Evapotranspiration	Calculated from pan data or from Linacre's equation	Calculated from pan data or from Hamon's formula	Calculated from pan data or from Linacre's equation
Pesticide sorption	Linear or Freundlich, two-site possible	Linear	Linear, time-dependent possible
Pesticide degradation	First-order kinetics, temperature- and moisture content-dependent chemical/biological	First-order kinetics, no dependence on temperature or moisture content	First-order kinetics, temperature- and moisture content-dependent, chemical/biological
Volatilisation	Yes	Yes	No
Simulation possible prior to application	Yes	Yes	No

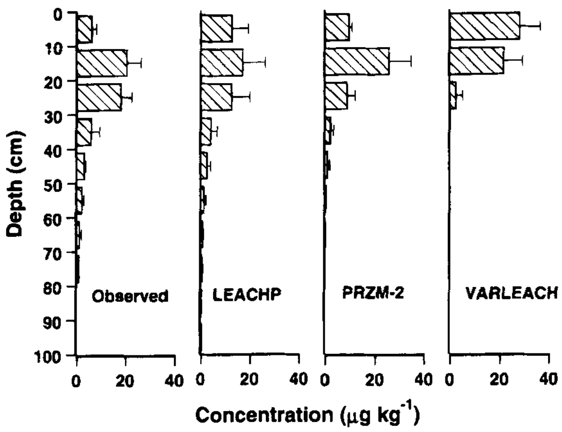

Fig. 1. Comparison between observed concentrations of the test chemical in soil 220 days after application (mean of three samples and one standard deviation) and those predicted by LEACHP, PRZM-2 and VARLEACH (mean of five simulations and one standard deviation).

the beginning of January reached a maximum of 0·6 μg litre^{-1} in March and then decreased rapidly to 0·2 μg litre^{-1} in the last soil-water sample taken on 23 May 1994. Detections of the test chemical in the first two samples of soil water collected after application have been omitted because there was no significant rainfall during the intervening period and the test chemical was also detected in the blank sample collected on the same dates. These detections were thought to be related to traces of chemical contaminating the outside of the sample bottles through contact with the soil and then being carried into the extraction procedure. Observed concentrations of the test chemical in soil water are means of 9 samples and Table 5 also gives the standard deviation. Replication was always very good and indicates that further sample contamination is unlikely to have occurred once significant rainfall had washed the initially large concentrations of test chemical from the soil surface. The results of soil sampling to 1 m depth on 8 June 1994 showed the movement of a broadening band of pesticide down the soil profile, with a maximum

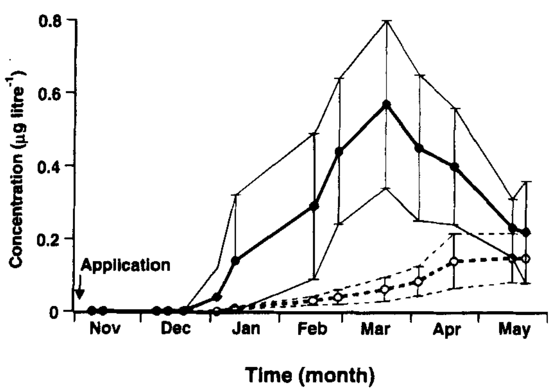

Fig. 2. Comparison between observed concentrations of the test chemical in soil water at 1 m depth (——; mean of nine samples ± one standard deviation) and those predicted by LEACHP (---; mean of five simulations ± one standard deviation).

residue of approximately 20 μg kg^{-1} at 10–20 cm depth. Data for soil residues are means from three profile pits and there was again remarkably good agreement between the replicates as indicated by the values for standard deviation. On 8 June 1994 (220 days after treatment), 37·1% of the test chemical applied remained in the soil profile and an effective first-order half-life for the field of 159 days was calculated and provided to the modellers as input. The general form of both the breakthrough curve for the test chemical and the pattern of residues down the soil profile suggests that by-pass flow was not a dominant process in this soil. Hence, the lack of any treatment of by-pass flow by the three models does not mean that they should be excluded from the present test.

There was a consistent difference in the ability of the three models to simulate the observed leaching of pesticide. This was reflected in the timing of breakthrough and maximum concentrations observed in soil water at 1 m depth as well as the depth of penetration of trace residues of pesticide in soil (see Table 6). Goodness-of-fit for leaching decreased in the order LEACHP >PRZM-2 >VARLEACH. The three models contain very different descriptions of water flow and/or solute transport (see Table 4) and the overall variation in predicted mobility is likely to be a reflection of these descriptions.

At the end of the experiment (220 days after treatment), the total residue of the test chemical in the top 1 m of soil was equivalent to 78·5 g ha^{-1}. There was again variation in the ability of the models to simulate this residue, with PRZM-2 generally giving the best results (Table 6). Mean results suggest that VARLEACH and LEACHP gave better simulations of the total residue than PRZM-2 (means from the five runs of 77·0, 73·6 and 66·5 g ha^{-1}, respectively), but there was much less variation between the five simulations with PRZM-2 (standard deviation 5·3 compared to 24·6 and 42·8 for VARLEACH and LEACHP, respectively). Although the half-life given for modelling was derived from the field experiment, several of the modellers decided to include dependency of rate of degradation upon soil temperature and moisture content in order to better simulate leaching over the whole experiment with LEACHP. For VARLEACH, it is not possible to run the model without selecting parameters to describe the dependence of degradation on soil conditions. This dependency was described by relating the calculated half-life to the mean soil temperature and moisture content over the study period, and will have introduced user-dependent variation into the modelling process. For example, simulation 5 with VARLEACH predicted larger total residues in soil 220 days after treatment than the other four simulations because degradation was allowed to vary around a reference temperature for the stated half-life of 15°C compared to reference temperatures of 7–10°C for the other four simulations.

TABLE 5

Comparison between Observed Concentrations of the Test Chemical (a) in Soil Water at 1 m depth (μg litre^{-1}) and (b) in Soil 220 Days after Treatment ($\mu g\ kg^{-1}$) and Those Predicted by Five Modellers using LEACHP, PRZM-2 and VARLEACH

	Observed		*Predicted by LEACHP*					*Predicted by PRZM-2*					*Predicted by VARLEACH*				
(a) *Date*	*Mean*	(*s.d.*)	*1*	*2*	*3*	*4*	*5*	*1*	*2*	*3*	*4*	*5*	*1*	*2*	*3*	*4*	*5*
10 Nov. 1993	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15 Nov. 1993	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9 Dec. 1993	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14 Dec. 1993	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21 Dec. 1993	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5 Jan. 1994	0	(–)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13 Jan. 1994	0·14	(–)	0·01	0·01	0	0·01	0·01	0	0	0	0	0	0	0	0	0	0
17 Feb. 1994	0·29	(0·20)	0·04	0·03	0·01	0·03	0·04	0	0	0	0	0	0	0	0	0	0
28 Feb. 1994	0·44	(0·20)	0·06	0·03	0·01	0·04	0·06	0·01	0	0·01	0	0	0	0	0	0	0
21 Mar. 1994	0·57	(0·24)	0·09	0·06	0·01	0·06	0·09	0·01	0	0·02	0	0	0	0	0	0	0
5 Apr. 1994	0·45	(0·20)	0·12	0·07	0·03	0·07	0·13	0·02	0	0·02	0	0	0	0	0	0	0
21 Apr. 1994	0·40	(0·16)	0·20	0·12	0·03	0·13	0·22	0·02	0	0·05	0	0	0	0	0	0	0
17 May 1994	0·23	(0·08)	0·22	0·14	0·04	0·16	0·18	0·02	0	0·10	0	0·01	0	0	0	0	0
23 May 1994	0·22	(0·14)	0·22	0·13	0·04	0·16	0·19	0·02	0	0·11	0	0·01	0	0	0	0	0

	Observed		*Predicted by LEACHP*					*Predicted by PRZM-2*					*Predicted by VARLEACH*				
(b) *Depth* (*cm*)	*Mean*	(*s.d.*)	*1*	*2*	*3*	*4*	*5*	*1*	*2*	*3*	*4*	*5*	*1*	*2*	*3*	*4*	*5*
0–10	4·6	(2·0)	8·4	13·5	2·9	18·2	18·4	10·3	9·0	9·9	7·3	8·9	24·9	25·6	26·0	20·2	42·3
10–20	19·6	(5·8)	10·6	19·0	4·1	25·4	25·0	27·2	19·5	14·0	37·6	29·0	21·0	17·7	22·0	12·8	33·7
20–30	18·3	(4·5)	7·7	11·8	2·6	17·4	21·5	10·3	9·5	11·2	2·9	8·1	1·1	0·7	7·0	0·5	1·2
30–40	4·3	(3·6)	2·8	3·1	0·7	5·1	7·6	2·3	1·2	3·5	0·2	1·0	<0·1	<0·1	<0·1	<0·1	<0·1
40–50	2·5	(0·6)	1·6	1·6	0·4	2·6	4·8	0·9	0·3	2·0	<0·1	0·3	<0·1	<0·1	<0·1	<0·1	<0·1
50–60	1·4	(0·9)	0·6	0·6	0·1	0·9	2·2	0·3	<0·1	0·8	<0·1	0·1	<0·1	<0·1	<0·1	<0·1	<0·1
60–70	1·0	(0·9)	0·3	0·3	0·1	0·4	1·3	0·1	<0·1	0·5	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1
70–80	0·6	(–)	0·2	0·2	<0·1	0·2	0·6	<0·1	<0·1	0·2	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1
80–90	<0·5	(–)	<0·1	<0·1	<0·1	<0.1	0·2	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1
90–100	<0·5	(–)	<0·1	<0·1	<0·1	<0.1	0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1	<0·1

TABLE 6
Summary of Observed Results from the Field Experiment and Those Predicted by Five Modellers Using LEACHP, PRZM-2 and VARLEACH

Result/Model output	*Observed value*	*Predicted value* 1	2	3	4	5
Maximum pesticide concentration at 1 m depth (μg litre^{-1})	0·57					
LEACHP		0·22	0·14	0·04	0·16	0·22
PRZM-2		0·02	0	0·11	0	0·01
VARLEACH		0	0	0	0	0
Maximum soil depth with residues > 0·5 μg kg^{-1} (cm)	70–80					
LEACHP		50–60	50–60	30–40	50–60	70–80
PRZM-2		40–50	30–40	60–70	20–30	30–40
VARLEACH		20–30	20–30	20–30	20–30	20–30
Total pesticide residue in soil after 220 days (g ha^{-1})	78·5					
LEACHP		48·3	75·2	16·4	105·3	122·6
PRZM-2		66·8	59·3	63·2	72·0	71·1
VARLEACH		70·5	66·0	82·5	50·3	115·8

PRZM-2 does not have a routine to describe changes in rate of pesticide degradation with varying soil temperature and moisture content, so that the variation between the five predictions for total residues of the test chemical in soil was much less than that for the other two models. It can be concluded that, even though modelling the effects of changes in soil temperature and moisture content on rate of pesticide degradation will give an improved simulation of reality if properly performed, this should be avoided for field-derived half-lives unless a recognised procedure for doing so is developed.

Although all modellers received the same information with which to select input parameters, no two simulations with any of the three models were identical. This was true even for the relatively simple model VARLEACH which only requires 20 parameters to be set to carry out a simulation. The user-dependence was found to be caused by a number of key input parameters which could not be derived from the experimental information provided and were thus open to considerable subjectivity according to the experience and knowledge of the individual modeller (Table 7). The subjective parameters for this series of simulations fall mainly into two categories. The first describes the initial state of the system to be modelled (e.g. soil moisture content and soil temperature). Such information is frequently lacking where experiments have been carried out for purposes other than modelling and must always be estimated where models are used predictively. Selection of these parameters reflected the experience of the individual modeller, so that the highest values for initial soil temperature were selected by the Italian group, whilst lower temperatures were selected by groups from

TABLE 7
Main Input Parameters Accounting for User-Dependence in Model Simulations (Values in Parentheses give the Range for the Five Simulations)

LEACHP	*PRZM-2*	*VARLEACH*
Dispersivity (10–100 mm)	Layer thickness (i.e. dispersivity—see Fig. 1)	Reference moisture content for degradation (0·15–0·25 g g^{-1})
Dependence of degradation on soil moisture content and temperature (none—dependent on both)	Rate of pesticide uptake by plants (none—transpiration*solution concentration)	Reference temperature for degradation (6·7–15°C)
Initial soil moisture content (0·15–0·25 g g^{-1})	Initial soil moisture content (0·16–0·25 g g^{-1})	Increase in pesticide half-life down the profile (1–6·5 times)
Initial soil temperature (4–18°C)	Equilibration period before pesticide application (0–10 months)	Initial soil moisture content (0.18–0·25 g g^{-1})
Air diffusion coefficient for the pesticide (4300–6700 cm^2 d^{-1})		
Equilibration period before pesticide application (0–10 months)		

Germany and the UK. Initial soil conditions can have a significant effect upon rates of degradation soon after application, particularly where no period before application is modelled to allow model conditions to equilibrate. For LEACHP, particular attention needs to be given to correctly setting the initial soil temperatures down the profile, as these are used to set the range over which soil temperature fluctuates for the whole simulation. The second main group of parameters were those resulting from modellers extrapolating beyond the information provided in order to better approximate their view of the field situation. These parameters included introducing a variable rate of degradation according to soil moisture content and temperature, varying rate of degradation down the soil profile, and accounting for uptake of pesticide by the plant.

Dispersivity is a very important parameter for modelling, and to a large extent accounted for differences in the amount of leaching predicted by the different users. In VARLEACH, dispersivity is introduced both through the definition of the mobile and immobile water categories and the interaction between them and numerically by defining the segment thickness used to divide the soil profile. The division between mobile and immobile water is fixed at 200 kPa and segment thickness is set at 1 cm, so that the amount of dispersion introduced into the system is effectively fixed for a given soil type. Dispersivity can also be introduced numerically into PRZM-2 and, although guidance suggesting limits for the range of appropriate segment thicknesses is provided, the actual values to be used must still be specified by the modeller. As illustrated in Fig. 3, the segment thickness selected by the five users varied considerably and this was reflected in a large variation in predictions for leaching. Simulation 4 had the smallest segment thickness (1 cm) in the topsoil and predicted the least leaching of the test compound (see Table 5) whilst simulation 3 had 5-cm segments all the way down the soil profile and predicted the greatest leaching. PRZM-2 also allows numerical dispersion to be

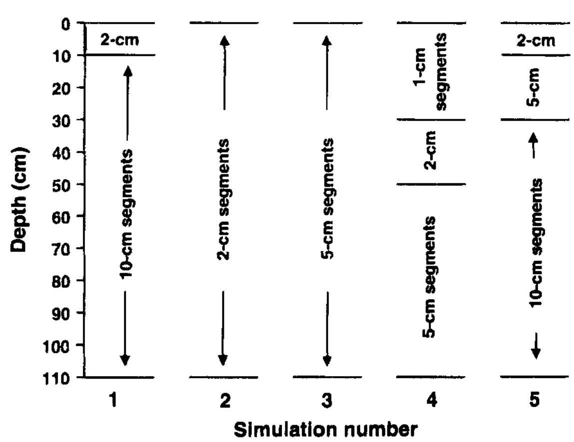

Fig. 3. Segment thickness selected by the five modellers to predict leaching using PRZM-2.

eliminated from the model and analytical dispersivity to be introduced, although the user manual advises against this unless experimental estimates for dispersivity are available. This method was chosen by one of the model users (simulation 3). Dispersivity is always an analytical component for LEACHP, with numerical dispersivity corrected for in the code. The values for dispersivity chosen by the users varied by a factor of 10 for the five simulations.

Changing the values of certain parameters from those supplied with the model can cause significant changes in modelling results which are not necessarily expected by the user. Simulation 3 with LEACHP predicted significantly smaller total residues of the test chemical in soil than the other model runs (see Table 5). This resulted mainly from a change in the value for the molecular diffusion coefficient of pesticides in soil from 4300 cm^2 day^{-1} which is supplied with example input files for LEACHP to 6700 cm^2 day^{-1} derived from the molecular weight of the test compound using Graham's law. Coupled with a high initial soil temperature, this change caused a large increase in the amount of pesticide volatilised, such that the total loss of the test chemical from degradation and volatilisation over the course of the experiment increased from 79·4% to 90·4%. This result demonstrates the importance of sensitivity analyses to effective model use as well as the problems which may arise from changing the values of input parameters from those supplied, and thus presumably used, by the model developer.

It is important to compare the uncertainty in predictions for pesticide fate likely to be introduced as a result of subjectivity in modelling with the uncertainty associated with measuring pesticide fate in the field.[10] Figure 1 compares observed and predicted residues of the test chemical in soil at the end of the experiment along with the standard deviation associated with each. As described above, there were differences in the reproducibility of predictions for total residues of the test chemical in soil for the three models, but there was little difference in the standard deviations associated with results from each model when the soil profile was broken down into 10-cm layers. The standard deviation as a proportion of the mean of the five simulations with each model generally increased down the soil profile, with ranges of 54–110, 13–108 and 30–131% for LEACHP, PRZM-2 and VARLEACH, respectively. The variability associated with modelling results was of the same order of magnitude as that associated with field results for which the standard deviation represented 21–92% of the mean of the three soil samples for each depth increment.

Figure 2 compares mean pesticide residues in soil water at 1 m depth and the associated standard deviation with predictions from LEACHP—the only one of the three models for which all five modellers predicted residues at this depth. Timing of breakthrough of pesti-

cide was well predicted by LEACHP, but the magnitude of the peak concentration was underestimated and its timing was delayed compared to observed results. Generally, the standard deviation for the five simulations was smaller than the discrepancy between observed and predicted data. By the end of the experiment, observed and predicted concentrations of pesticide were very similar and the standard deviations associated with measured and simulated concentrations were of a similar order of magnitude.

5 CONCLUSIONS

The ring test shows that modelling results for the same scenario and model can vary between users. In this case, the variation between five simulations was similar to that associated with the measurements of pesticide behaviour in the field. This user-dependence of modelling has not previously been considered, but should be an important component of evaluating any model output. For example, much effort is currently targeted at model validation and defining the range of that validity. To date, this effort has involved comparison between a given set of field observations and a single model simulation or a range of simulations carried out by a single user. Even where predicted results give an acceptably accurate simulation of field behaviour, the findings of the ring test suggest that claims of validity will be misleading unless it can be proved that similarly accurate results would be obtained by a number of independent users.

Model developers should be encouraged to reduce model subjectivity by decreasing the number of parameters which are not readily measured or available in the literature and providing detailed guidance for selection of such parameters as cannot be eliminated. The US Environmental Protection Agency has recently produced such a guidance table for the models PRZM-2 and EXAMS (Wadley, A.M.A., 1995, pers. comm.). The scientific basis for models of pesticide fate and behaviour needs to be continuously reviewed and developed and current work on describing the process of macropore flow is an example.[11] However, this development needs to be accompanied by efforts to improve the overall user-friendliness of current models, with particular emphasis upon the guidance available to ensure appropriate and consistent selection of input parameters. Subjectivity is clearly inherent in much of the modelling for pesticide fate and behaviour carried out at present, and it is likely that, without this, the modelling process would lose much of the flexibility which makes it such a powerful tool. However, the present exercise demonstrates that constraints need to be imposed upon that subjectivity where model output is to be used to support the broad range of decisions which are made with regard to pesticides in the environment. Model output must be accompanied by a detailed list of the input parameters used for simulations along with a brief description of the rationale for parameter selection in order to allow proper evaluation of the results obtained.

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